

Delaval, Jan

113779

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Jan,

Please search claims 1 with a look at claims 2-11 which clarify the issue.

1. A method for generating a protozyme (or enzyme) , said method comprising:
 - a) identifying a suitable protein scaffold lacking a desirable enzyme-like activity;
 - b) inputting a protein backbone structure of said protein scaffold into a computer, wherein said backbone structure has variable residue positions ;
 - c) inserting an active site domain into said scaffold;
 - d) applying at least one protein design cycle; and
 - e) generating a set of candidate variant proteins with putative enzyme-like activity.
2. A method according to claim 1 wherein said insertion step is done at the same time as said protein design cycle.
3. A method according to claim 1 wherein said insertion step is done prior to said applying step.
4. A method according to claim 1 wherein said insertion step is done after said applying step.
5. A method according to claim 1 wherein said insertion step comprises the use of at least one high energy state rotamer.
6. A method according to claim 1 further comprising applying a second protein design cycle prior to said generating step.
7. A method according to claim 1 wherein said active site domain catalyzes a known enzymatic reaction.
8. A method according to claim 1 wherein said active site domain catalyzes an unknown enzymatic reaction.
9. A method according to claim 1 wherein said active site domain is a ligand binding domain.
10. A method according to claim 1 wherein said protein design cycle comprises a DEE computation
11. A method according to claim 1 wherein said protein design cycle includes the use of at least one scoring function.

Thanks a lot

Michael